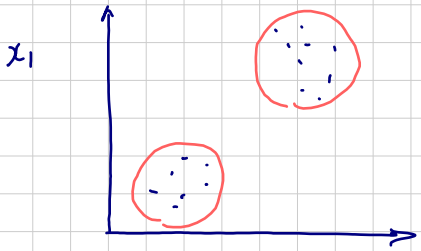
Machine Learning Week 8

Unsupervised Learning



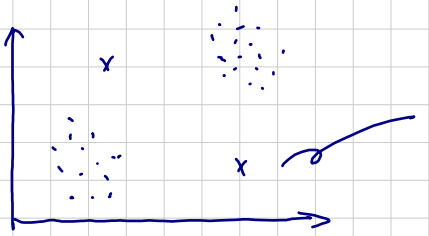
group / clustering:
find some structures

1. Clustering

Training set $\{ x^{(1)}, x^{(2)}, \cdots, x^{(m)} \}$

Applications
- market segmentation
- social network analysis
- organize computer clusters
- astronomical data analysis

2. K-means Algorithm



cluster centroids. (randomly initiated)

Step (1) Cluster assignment.
- binary assignment of datasets depending on proximity.

(2) Move centroid.
- move to "mean" of location in all labelled

re-colour.

[Input].

① K (number of clusters)

② Training set $\{x^{(1)}, x^{(2)}, \cdots, x^{(m)}\}$

$x^{(i)} \in \mathbb{R}^n$ [drop $x_0 = 1$ convention]

[Algorithm]

Randomly initialize K cluster centroids μ_k, $k = 1 \cdots K$

do {

for $i = 1 \cdots m$.

cluster assignment: $c^{(i)} := \min_k \| x^{(i)} - \mu_k \|^2$.

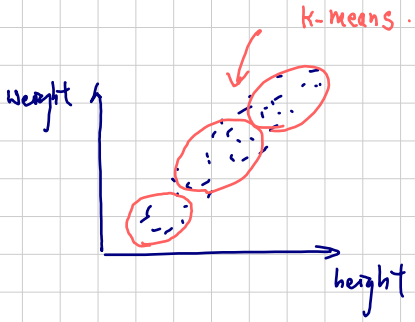
for $k = 1 \cdots K$

move centroid: $\mu_k := \text{mean}(\text{pts assigned to cluster } k)$

$\in \mathbb{R}^n$

3. K-means for non-separated clusters.

T-shirt sizing



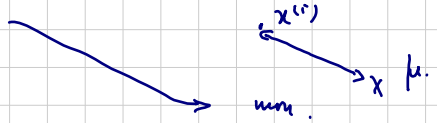
Optimization objective

K-means optimization objective.

- $c^{(i)}$: index.
- μ_k : cluster centroid k $\quad \in \mathbb{R}^n$
- $\mu_{c^{(i)}}$ = cluster centroid of cluster to which $x^{(i)}$ has been assigned.

$$J(c^{(1)}, \dots, c^{(m)}, \mu_1 \cdots \mu_K) = \frac{1}{m} \sum_{i=1}^{m} \| x^{(i)} - \mu_{c^{(i)}} \|^2$$

$$\min_{\substack{c^{(1)} \cdots c^{(m)} \\ \mu_1 \cdots \mu_K}} J(\cdots)$$



[Algorithm]

Randomly initialize K cluster centroids μ_k, $k = 1 \cdots K$

do {

for $i = 1 \cdots m$.

cluster assignment:

$$c^{(i)} := \min_k \| x^{(i)} - \mu_k \|^2$$

Minimize $J(\cdots)$ wrt. $c^{(1)} \cdots c^{(m)}$. [holding $\mu_1 \cdots \mu_K$]

for $k = 1 \cdots K$

move centroid:

$\mu_k :=$ mean (pts assigned to cluster k)

$\in \mathbb{R}^n$

Min. w.r.t. $\mu_1 \cdots \mu_K$

Random Initialization

Rules.

(1) $K < m$

(2) Randomly pick K training examples

(3) set μ_k = examples

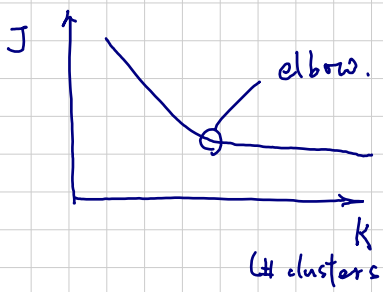
- Might have different clustering (local optimum) ⟶ try different random initialization.

- Implementation.

```
for i=1 ... 1000 {

    randomly initialize K-means
    run K-means. get c^(1) ... c^(m), μ_1 ... μ_K

    complete cost function (distortion)
        ↳ J( c^(1), ..., c^(m), μ_1 ... μ_K )

}

Pick one with lowest cost J.
```

Choose K

1. Elbow method:

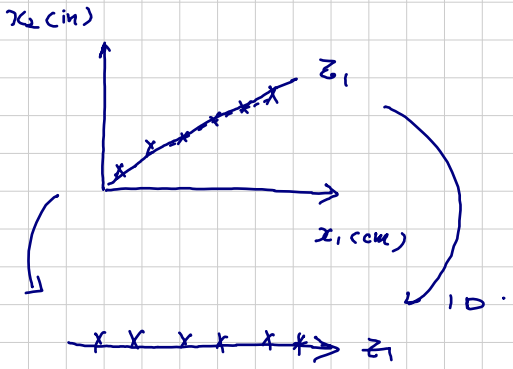


2. Pre-defined (t-shirt sizes: 2... 5).

Dimensionality Reduction

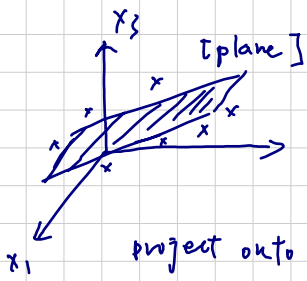
1. Motivation I : Data compression

- Redundent data dimension (cm, inch, ...)

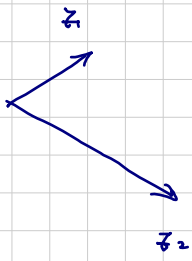


ex. 3D → 2D .

$x^{(i)} \in \mathbb{R}^3$



→ need 2-axis for plane



project onto a plane

$z^{(i)} \in \mathbb{R}^2$. $\begin{pmatrix} z_1^{(i)} \\ z_2^{(i)} \end{pmatrix}$

(correlation approximation)

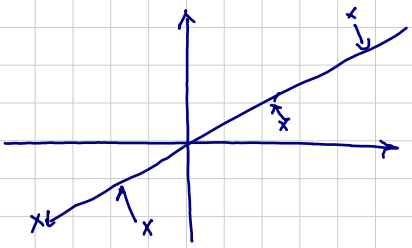
procedure. project data to one less dimension. → re-coordinate.

2 Motivation II: Data visualization.

. Combine certain features (correlated) . $x \rightarrow z$

(500) (2)

Principal Component Analysis



Try to find a lower dimension surface to min. projection error.

→ perform mean normali. and feature scaling.

- Principal Component Analysis [PCA] problem formulation

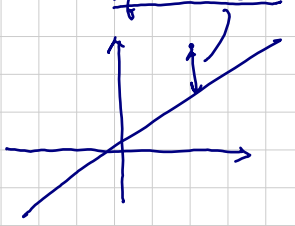
  2 → 1
  - find dir. vector $u^{(1)} \in \mathbb{R}^n$ onto which data projects

  n → k
  - find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which data projects.

    [project data to the linear subset span by $\{u^{(i)}\}_1^k$]

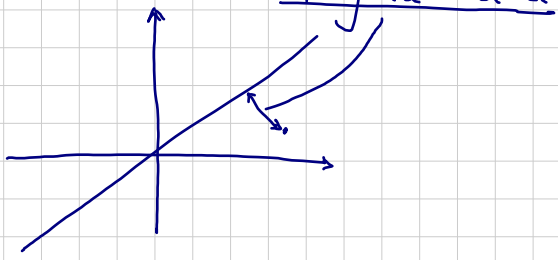
- . linear regression

  min. squared error



PCA.

min. orthogonal distance



Applys to higher dimension.

Principal component analysis component.

- Data preprocessing
  - mean normalization
  - feature scaling

- Reduction $x^{(i)} \in \mathbb{R}^2 \longrightarrow z^{(i)} \in \mathbb{R}$ [2D to 1D]

- Mathematical derivation (complicated)

Algo.

① Reduce data from $\mathbb{R}^n$ to $\mathbb{R}^k$

Compute "covariance matrix" Sigma. $\in \mathbb{R}^{n \times n}$ $(n \times 1)(1 \times n)$

$$\Sigma = \frac{1}{m} \sum_{i=1}^{n} [x^{(i)}][x^{(i)}]^T = \left(\frac{1}{m}\right) \cdot X^T \cdot X.$$

$X = \begin{pmatrix} - & - \\ - & - \end{pmatrix}$ (n)

Compute "eigenvectors" of matrix Σ → singular value decomposition

$[U, S, V] = \text{svd}(\text{Sigma})$

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \cdots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

first k vectors: $u^{(1)} \cdots u^{(k)}$

② Projection.

$$U_{\text{reduce}} = \begin{bmatrix} | & & | \\ u^{(1)} & \cdots & u^{(k)} \\ | & & | \end{bmatrix} \in \mathbb{R}^{n \times k}$$

$$z^{(i)} = U_{\text{red}}^T \cdot x^{(i)} = \begin{pmatrix} (k \times n) \\ - u^{(1)} - \\ \vdots \\ - u^{(k)} - \end{pmatrix} \overset{(n \times 1)}{x^{(i)}} = (k \times 1)$$

Reconstruction from Compressed Representation

$z = U_{reduce}^T x$. $\quad z \in \mathbb{R} \longrightarrow x \in \mathbb{R}^2$?

$x \approx x_{approx} = \underbrace{U_{reduce}}_{(n \times k)} \cdot \underbrace{z}_{(k \times 1)}$.

Choosing k (# of principal components)

- Average Square projection error $\frac{1}{m} \sum_{i=1}^{m} \| x^{(i)} - x_{approx}^{(i)} \|^2$
- Total variation in data $\frac{1}{m} \sum_{i=1}^{m} \| x^{(i)} \|^2$
- Typically, choose k to be min s.t.

$$\frac{\frac{1}{m} \sum_{i=1}^{m} \| x^{(i)} - x_{approx}^{(i)} \|^2}{\frac{1}{m} \sum_{i=1}^{m} \| x^{(i)} \|^2} \leq 0.01 \quad (1\%) \qquad [*]$$

"99% variance retained"

- Algorithm.

1) try PCA with $k=1$
2) Compute $U_{reduce}, z^{(1)}, z^{(2)}, \dots z^{(m)}$
   $x_{approx}^{(1)} \cdots x_{approx}^{(m)}$
3) check $[*]$
4) $k = k+1 \longrightarrow 2$

- $[U, S, V] = svd(Sigma)$

$n \times n$ diagonal, $S = \begin{pmatrix} S_{11} & & 0 \\ & \ddots & \\ 0 & & S_{nn} \end{pmatrix}$

For given k, $(*)$ can be computed as $\left(1 - \frac{\sum_{i=1}^{k} S_{ii}}{\sum_{i=1}^{n} S_{ij}}\right)$

$\sum_{i=1}^{n} S_{ij} \geq 0.99$

Advice for applying PCA

Supervised learning speed up

$x^{(i)} \in \mathbb{R}^{10000}$

$(x^{(1)}, y^{(1)}) \dots (x^{(m)}, y^{(m)})$

Extract inputs:

Unlabelled dataset $x^{(1)}, x^{(2)} \dots x^{(m)} \in \mathbb{R}^{10000}$

$\downarrow$ PCA (defined running only on training set)

$z^{(1)} \dots z^{(m)} \in \mathbb{R}^{1000}$

New training set

$(z^{(1)}, y^{(1)}) \dots (z^{(m)}, y^{(m)}) \rightarrow$ train. $h_\theta(z) = \frac{1}{1+\exp(-\theta^T z)}$

Example

$x \rightarrow z \rightarrow h(z)$

(prediction)

Application

- Compression → choose k by % variance retained.
- Visualization → $k = 2, 3$

What not to do → prevent overfitting

- Use $z^{(i)}$ instead of $x^{(i)}$. reduce # of features from n to k.

→ fewer features, less likely to overfit. (Why → PCA throws away information w/o knowing y?

- Should use λ.

PCA usage.

Design of ML sys.?

- get training set
- [- run PCA reduce $x^{(i)} \rightarrow z^{(i)}$] do w/o this step first.
- train logistic.
- test set